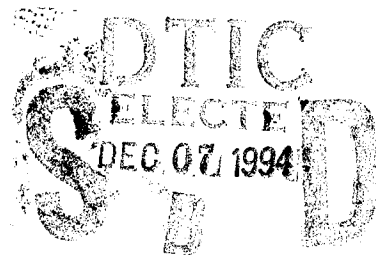


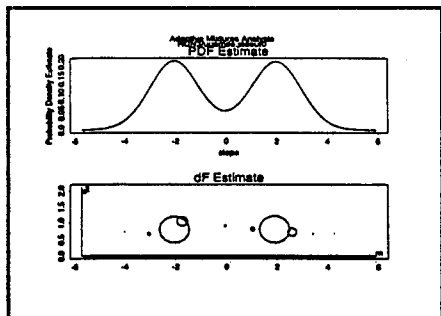
A Method to Determine the Structure of an Unknown Mixture Using the Akaike Information Criterion and the Bootstrap

*Jeffrey L. Solka, Edward J. Wegman, Carey E. Priebe,
Wendy L. Poston and George W. Rogers*

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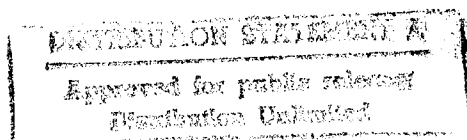
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A Method to Determine the Structure of an Unknown Mixture Using the Akaike Information Criterion and the Bootstrap

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ABSTRACT

Given i.i.d. observations $x_1, x_2, x_3, \dots, x_n$ drawn from a mixture of normal terms one is often interested in determining the number of terms in the mixture and their defining parameters. Although the problem of determining the number of terms is intractable under the most general assumptions there is hope of elucidating the mixture structure given appropriate caveats on the underlying mixture. This paper examines a new approach to this problem based on the use of Akaike Information Criterion (AIC) based pruning of data driven mixture models which are obtained from resampled data sets. Results of the application of this procedure to artificially generated and real world data sets are provided.

1. Introduction

Given $X = \{\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n\}$ where each \mathbf{x}_i is d dimensional and i.i.d. according to an unknown density $f_0(\mathbf{x})$ one is often interested in estimating $f_0(\mathbf{x})$. This problem occurs in such areas as exploratory data analysis, classification, and regression. There are a variety of approaches to the multivariate density estimation problem (Scott, 1992).

An often used parametric approach is that of finite mixture models (Everitt and Hand, 1981) in combination with the expectation maximization (EM) method of Dempster, Laird, and Rubin (1977). One difficulty with this tactic is that one needs some idea as to the appropriate number of terms in the mixture model as well as the approximate parameter values. Given this information the EM algorithm is guaranteed to converge to at least a local maxima in the likelihood surface.

Some of the previous nonparametric approaches include histograms (Sturges, 1926), frequency polygons (Scott, 1985a), adaptive histograms (Wegman, 1970), average shifted histograms (Scott, 1985b), and kernel estimators (Silverman, 1986). These approaches are beneficial in that they possess nice asymptotic consistency properties, robustness with regard to nonnormality, and fewer parameters to estimate which implies better estimates in the finite sample regime. They are at a disadvantage as compared to the mixture model approach when it is suspected that the unknown true density is a mixture of a number of terms and one would like to estimate the posteriori probability of underlying term membership for an unlabeled observation.

This type of problem exists in the areas of medical diagnosis and image processing. In medical diagnosis the term membership may play an important role in identification of the

of terms which is based on the use of the Akaike Information Criterion (AIC) is performed to obtain a model that not only matching the underlying distribution in a functional sense but also with regard to model complexity. Subsequent sections will detail how well that our pruning based procedure meets these goals.

The AIC was originally developed as a tool to choose between two statistical estimators of differing complexities (Akaike, 1972). The AIC is written as a function of the likelihood L and number of free parameters M in a model as follows

$$AIC(\hat{f}) = -2\ln(L) + 2M.$$

In Akaike's original paper the AIC was applied to time series analysis, but subsequent work has applied the technique to ISODATA based (Carman and Merickel, 1990) and general clustering (Bozdogan and Sclove, 1984), and finite mixture analysis (Liang Jaszczak, and Coleman, 1992).

We have developed a new approach to finite mixture determination which employs AIC based pruning of AMDE estimates. This approach differs from the work of Liang in two ways. Liang chooses to make an initial guess as to the appropriate complexity of the data's finite mixture model and then adjusts the number of terms in the model up and down by adding and removing a term until no further improvement is possible. Our approach begins with an over determined data driven model that is produced by the AMDE procedure and then uses AIC in combination with the expectation maximization technique to prune superfluous terms from the model. So whereas Liang's approach adds and subtracts terms to the model our approach just removes terms. The second difference is that where Liang's approach is to produce a single best solution to the finite mixtures question our approach produces a distribution of model complexities from which estimates of the appropriate model complexity can be made.

Section 2 develops the methodology for term pruning in the case of finite mixtures models obtained from finite sample application of the adaptive mixtures procedure. Section 3 presents results indicating that we can improve upon an overdetermined mixture model and in some cases determine the true model complexity. Section 4 concludes with a discussion of the relevance of these results.

2. Approach

Our approach combines elements of nonparametric density estimation, parametric density estimation, and information based pruning. The nonparametric AMDE is used as the starting point of our procedure. We begin our discussions with an overview of AMDE.

2.1 Adaptive mixtures density estimation

Given an unknown distribution $f_0(\vec{x})$ we seek to model the distribution using $\hat{f}(\vec{x})$ defined by

$$\hat{f}(\vec{x}; \Psi) = \sum_{i=1}^g \hat{\pi}_i K(\vec{x}; \hat{\theta}_i), \quad (1)$$

where K is some fixed density parameterized by $\hat{\theta}_i$, and $\hat{\Psi} = (\hat{\pi}_1, \hat{\theta}_1, \hat{\pi}_2, \hat{\theta}_2, \dots, \hat{\pi}_g, \hat{\theta}_g)$. The $\hat{\pi}_i$'s are referred to as the mixing proportions. (We can assume for much of what follows that K is taken to be the normal distribution, in which case $\hat{\theta}_i$ becomes $\{\hat{\mu}_i, \hat{\Sigma}_i\}$.) In the simplest case the mixture is assumed to have a single term and the parameters that need to be estimated are the mean and covariance of the distribution.

The basic stochastic approach to parameter estimation is to recursively update the estimate $\hat{\Psi}$ of the true parameters Ψ_0 based on the latest estimate $\hat{\Psi}_t$ and the newest data

point \hat{x}_{t+1} . That is,

$$\hat{\Psi}_{t+1} = \hat{\Psi}_t + \Phi_t(\hat{x}_{t+1}; \hat{\Psi}_t) \quad (2)$$

for some update function Φ_t . The specific form of the update equation that we use is the one suggested by Titterton (1984). If we let $I(\Psi)$ be the Fisher information then the version of the recursive update formula we will use is

$$\hat{\Psi}_{t+1} = \hat{\Psi}_t + (nI(\hat{\Psi}_t))^{-1} \left(\frac{\partial}{\partial \hat{\Psi}} \right) \log \hat{f}(\hat{x}_{t+1}; \hat{\Psi}_t) \quad (3)$$

where the derivatives represents the vector of partial derivative with respect to the terms of $\hat{\Psi}$.

In the case of mixtures of multivariate normals we may write the recursive update equations as

$$\hat{\tau}_{n+1}^{(i)} = \frac{\pi_n^{(i)} \hat{f}^{(i)}(\hat{x}_{n+1}; \hat{\theta}_n)}{\sum_{i=1}^g \pi_n^{(i)} \hat{f}^{(i)}(\hat{x}_{n+1}; \hat{\theta}_n)} \quad (4)$$

$$\hat{\pi}_{n+1}^{(i)} = \hat{\pi}_n^{(i)} + \frac{1}{n} \left(\hat{\tau}_{n+1}^{(i)} - \hat{\pi}_n^{(i)} \right) \quad (5)$$

$$\hat{\mu}_{n+1}^{(i)} = \hat{\mu}_n^{(i)} + \frac{\hat{\tau}_{n+1}^{(i)}}{n \hat{\pi}_n^{(i)}} \left(x_{n+1} - \hat{\mu}_n^{(i)} \right), \text{ and} \quad (6)$$

$$\hat{\Sigma}_{n+1}^{(i)} = \hat{\Sigma}_n^{(i)} + \frac{\hat{\tau}_{n+1}^{(i)}}{n \hat{\pi}_n^{(i)}} \left[\left(\hat{x}_{n+1} - \hat{\mu}_n^{(i)} \right) \left(\hat{x}_{n+1} - \hat{\mu}_n^{(i)} \right)^T - \hat{\Sigma}_n^{(i)} \right]. \quad (7)$$

This is where $\hat{\tau}_{n+1}^{(i)}$ is the estimated posteriori probability of \hat{x}_n belonging to the i th term

of the mixture, $\hat{\pi}_{n+1}^{(i)}$ is the estimated mixing coefficient, $\hat{\mu}_{n+1}^{(i)}$ is the d dimensional estimated mean, and $\hat{\Sigma}_{n+1}^{(i)}$ is the dxd estimated covariance matrix of the ith term.

The adaptive mixtures density estimation (AMDE) stochastic approximation approach is to recursively update $\hat{\Psi}$, the estimate of the true parameters Ψ_0 , while at the same time providing the capability to expand the extent of the parameter space $\hat{\Psi}$ if dictated by the underlying complexity of the data. We note that in the AMDE case our parameter space $\hat{\Psi}$ is given by $\hat{\Psi} = (\hat{\pi}_1, \hat{\theta}_1, \hat{\pi}_2, \hat{\theta}_2, \dots)$. The procedure

$$\hat{\Psi}_{t+1} = \hat{\Psi}_t + A \cdot U_t(\hat{x}_{t+1}; \hat{\Psi}_t) + B \cdot C_t(\hat{x}_{t+1}; \hat{\Psi}_t, t), \quad (8)$$

is used to recursively update the density where $A = [1 - P_t(\hat{x}_{t+1}; \hat{\Psi}_t)]$, and $B = P_t(\hat{x}_{t+1}; \hat{\Psi}_t)$. P_t represents a possibly stochastic create decision and takes on values 0 or 1. U_t updates the current parameters using equations (4-7) while C_t adds a new term to the model. As is implicit in the equation, the decision to add a new term is a function of the current data point, our current estimation of the parameters, and time. The time dependence is important in those cases that we wish to anneal the probability of creation as a function of training time. The models produced by the AMDE procedure are good functional estimates, but are typically overdetermined with regard to the number of terms.

2.2 Approaches to AIC based pruning of AMDE generated mixture models

Previous work in the literature has examined the application of the AIC to the determination of the number of terms in a finite mixture (Liang, Jaszczak, and Coleman, 1992). The AIC/n estimates -2 times the expected value of the log likelihood of the estimated model (Akaike, 1972)

$$\frac{AIC}{n} = -2E[\int f_0 \log \tilde{f}]. \quad (9)$$

AIC is defined in terms of likelihood, L, and the number of free parameters in the model,

M, as

$$AIC(\hat{f}) = -2\ln(L) + 2M = -2\ln[\hat{f}(\mathbf{x})] + 2M. \quad (10)$$

One uses the AIC to choose between models of differing complexities by selecting the model with the minimum AIC. This choice is equivalent to maximizing the mean likelihood of the model.

Using this idea as a starting point we have developed a procedure that uses a single or set of adaptive mixtures density estimates and produces a pruned model with a lower complexity. This procedure uses AIC to evaluate the appropriateness of lower complexity models that have been subjected to the iterative EM method. In the iterative EM method the update equation takes the form

$$\hat{\Psi}_{t+1} = \hat{\Psi}_t + \Phi(\vec{X}; \hat{\Psi}_t), \quad (11)$$

where Φ is the update function and \vec{X} is the set of observations. In the case of mixtures of multivariate normals we may write the iterative update equations as

$$\hat{\tau}_{ij} = \frac{\hat{\pi}_i \hat{f}_i(\mathbf{x}_j; \hat{\theta})}{\sum_{i=1}^g \hat{\pi}_i \hat{f}_i(\mathbf{x}_j; \hat{\theta})} \quad (12)$$

$$\hat{\pi}_{ij} = \sum_{j=1}^n \frac{\hat{\tau}_{ij}}{n} \quad (13)$$

$$\hat{\mu}_i = \frac{\sum_{j=1}^n \hat{\tau}_{ij} \mathbf{x}_j}{n \hat{\pi}_i}, \text{ and} \quad (14)$$

$$\hat{\Sigma}_i = \sum_{j=1}^n \frac{\hat{\tau}_{ij} (x_j - \hat{\mu}_i) (x_j - \hat{\mu}_i)^T}{n \hat{\pi}_i} \quad (15)$$

This is where $\hat{\tau}_{ij}$ is the estimated posteriori probability that x_j belongs to term i , $\hat{\pi}_{ij}$ is the estimated mixing coefficient, $\hat{\mu}_i$ is the d dimensional estimated mean vector, and $\hat{\Sigma}_i$ is the $d \times d$ estimated covariance matrix for the i th term.

The steps in our pruning procedure are as follows.

Step 1 - Obtain \hat{f}_g an initial adaptive mixtures approximation to f_0 containing g terms.

Step 2 - Compute the AIC of each of the $g-1$ term models after application of the EM method of equations (12-15) to each of the models.

Step 3 - If $AIC(\hat{f}_{g-1}) < AIC(\hat{f}_g)$ for one of the $g-1$ term models then the pruning process is repeated using this model.

Step 4. Repeat this process of pruning and expectation maximization until no further improvement is possible.

It is important to point out that at each pruning step the remaining terms $\hat{\pi}_i$'s are updated based on their Mahalonobis distance to the pruned term prior to updating with the EM method.

Figure 1 illustrates the pruning process. The log likelihood for the true model, the original ten term model, and the pruned and subsequently expectation maximized models are plotted. In this case the process was able to reduce a ten term model of the mixture $.5N(-2,1) + .5N(2,1)$ to the appropriate two term model. This case will be discussed in Section 3.

[FIGURE 1 SHOULD GO ABOUT HERE]

3. Results

This pruning procedure was tested on data sets drawn from two different bimodal two term distributions, one four mode four term distribution, a standard unimodal normal distribution, and the Buffalo snowfall data (Parzen, 1979), see Figure 2. In each simulated data case 10,000 points were drawn from each distribution. The snowfall data consisted of 63 points.

Twenty-five bootstrap resamples were extracted from each of the data sets using their empirical distributions (Efron and Tibshirani, 1993). These resamples are used in a way that is slightly different from the standard procedure. In standard bootstrapping one uses the resamples to estimate the standard error of a statistic whose standard error is not available in closed form. Our goal in bootstrapping is the production of a distribution on the number of terms in the models after AIC based pruning. This distribution can then be used to estimate the number of terms in the true model.

An up to ten term adaptive mixtures model was created for each of the resampled data sets. Each of these models were then subjected to the AIC based pruning process. This process provides a model complexity distribution based on the data set.

[FIGURE 2 SHOULD GO ABOUT HERE]

In Figures 3a and 3b we present adaptive mixtures solutions for two of the resamplings of the data set drawn from $\alpha(x) = .5 \cdot N(-2, 1) + .5 \cdot N(2, 1)$. We have included dF space plots along with the standard functional representation of the distributions. dF space plots are an effective way to display the terms in a mixture. Each term $\pi_i N(\mu_i, \sigma_i^2)$ is plotted as a circle whose radius is proportional to π_i and whose center is given by (μ_i, σ_i^2) . Where it is hard to

discern the distributional structure from a standard function plot it is quite easy in a dF space plot. We notice that the terms in each of the two solutions are markedly different. This phenomena falls under the adage that there is "more then one way to skin a cat" when producing a functional estimate. We also notice that there are more then the "theoretical" number of terms needed. Each of the models is made up of ten terms. The occurrence of a matching number of terms in each model is the result of our initial constraint on the model complexity. It is important to note that though the terms are different in each solution the location and number of modes is not and that there are terms that are superfluous to the minimal representation of the distribution.

[FIGURE 3 SHOULD GO ABOUT HERE.]

Table 1 illustrates the results of the pruning process. For each of the five distributions we have listed the number of terms in the final pruned models for each of the twenty-five resamples. In case a the procedure converged to the correct solution 11 of 25 times, 7 of 25 times in case b, 17 of 25 times in case c, and 3 of 25 times in case d. The procedure converged to a 3 term solution 4 of the 25 times in the case of the snowfall data. The appropriate solution for the case of the snowfall data will be the subject of later discussions.

[TABLE 1 SHOULD GO ABOUT HERE.]

We may estimate the model complexity through the use of statistical measures on this distribution. For example one could choose the minimal order statistic as the measure of the number of terms in the minimal complexity mixture model that characterizes the data. This choice has the advantage that it represents the lowest complexity model obtainable from the procedure. Alternatively one could use the expected value of the distribution. This choice indicates the average complexity of the mixture models that represent the data set.

Table 2 presents the average L_1 error between the true mixture model and the pruned model for each of the first 4 cases for each of the obtained model complexities. No L_1 results were provide for the snowfall data since the true underlying model is unknown. It is encouraging to note that in each case the minimum average error occurs at the appropriate level of model complexity.

[TABLE 2 SHOULD GO ABOUT HERE.]

The number of modes in the snowfall data has been the topic of continued debate throughout the history of density estimation. Arguments have been made in favor of trimodal (Scott, 1992) and unimodal structure (Scott 1994). In Figure 4a we compare the output of the pruning process for one of the 3 term models to a standard kernel estimator with a bandwidth of 6. The bandwidth of 6 was chosen as an appropriate setting to illustrate the trimodality of the data (Silverman, 1986). The 3 term model has been expectation maximized against the original data in order to make a fair comparison between the two. We note that the two models are very similar in character and specifically with regard to the mode placement. In fact if we drop the bandwidth down to 4 we can obtain a solution that is even closer in character to our mixture model, see Figure 4b.

[FIGURE 4 SHOULD GO ABOUT HERE]

The last thing left to be discussed is the output of the pruning procedure. In Figures 5 a, b, c and 6 a and b we present an expectation maximized adaptive mixture solution along with the output of pruning this solution. We notice that the number of terms in the solution has been reduced from ten to the appropriate number in each case. We also notice that the terms left from the process are in approximately the correct location and have about the right mixing coefficients and variances.

[FIGURES 5 AND 6 HERE]

4. Conclusions

The AMDE procedure provides a data driven method for obtaining a good mixture model density estimate. The convergence properties of the procedure tend to guarantee that the model will be of higher complexity than the true density if the latter is a finite mixture. The exceptions to this occur when the sample size is small enough that too few terms are created by the AMDE. The AMDE thus provides a useful mixture model estimate of an unknown density.

The AIC provides a convenient tool for evaluating appropriate model complexity. It serves as a good “rule of thumb” in choosing between models. Under appropriate conditions it has the capability to help reveal the underlying mixture which generates the data set.

In many cases we have reason to believe that the unknown density is a mixture model but of unknown complexity. Then we are often interested in the structure of the underlying mixture model. It is in this case that AIC based pruning can be used to find not only an “optimal” model but also a distribution of pruned models which provides some knowledge about the true density.

In this paper we have presented a new technique to help determine the unknown structure of a mixture model. This technique uses a set of adaptive mixture solutions that have been subject to AIC based pruning to help determine the minimum complexity mixture model that best characterizes the data. The goal of this technique is the production of a more parsimonious mixture model of an unknown distribution.

This approach embodies the spirit in which the AIC should be used in that one is comparing two maximum likelihood solutions. There is a penalty with regard to computational complexity that occurs in the production of expectation maximized models at each step of the pruning process. However the pruning procedure is highly parallel in nature and we would expect substantial speedups on a MIMD machine.

Future work will focus on extending this technique to multivariate distributions, on a more in-depth analysis of the theoretical underpinnings of the approach, and on parallelization of the procedure. We also plan to pursue better term creation techniques within the AMDE framework. Finally we hope to produce an AMDE like estimator that uses term creations and annihilations.

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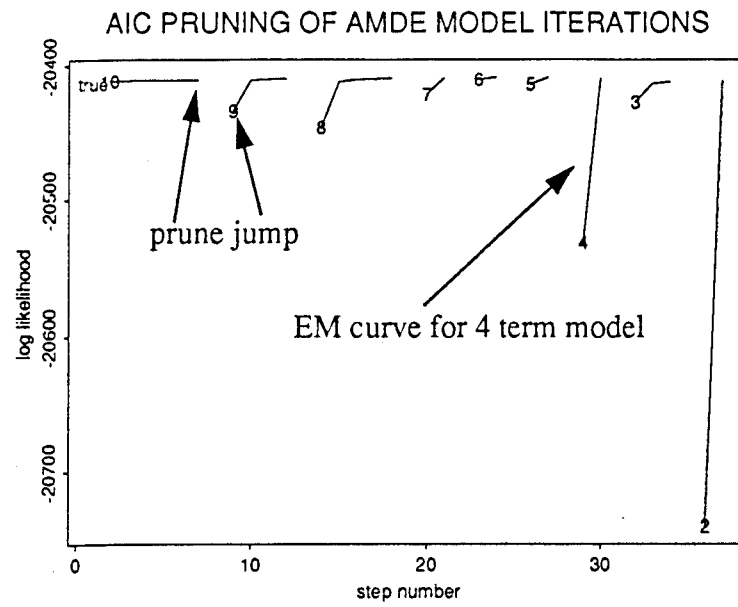
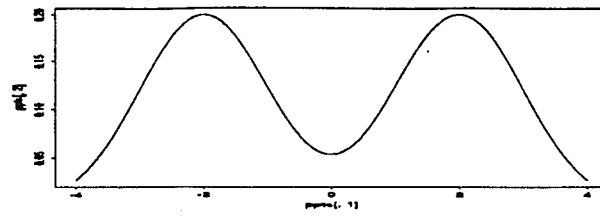
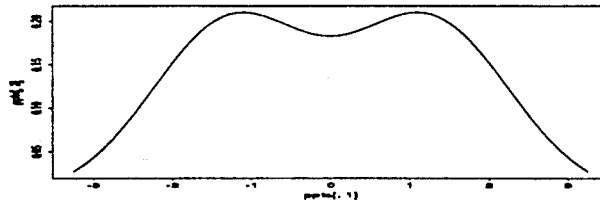


Figure 1

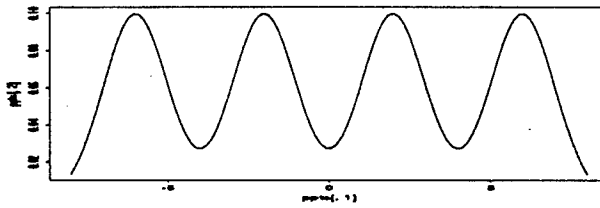
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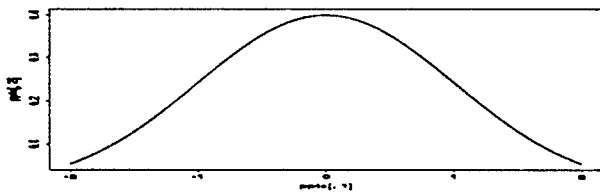
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Case c



Case d



Case e

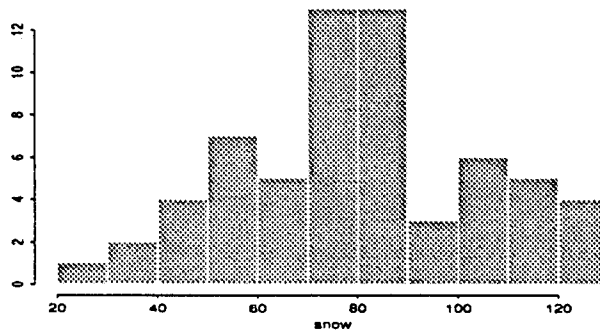
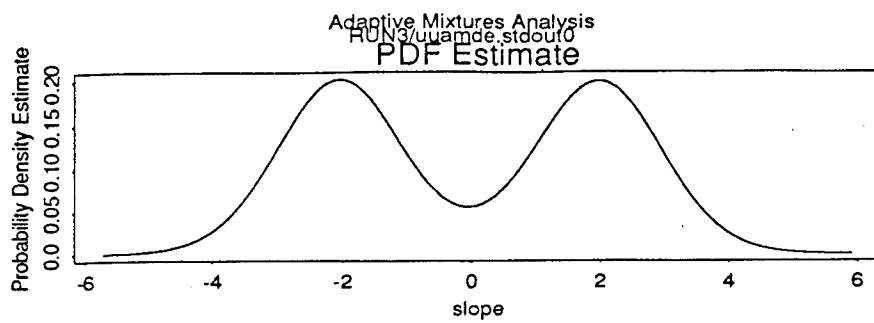
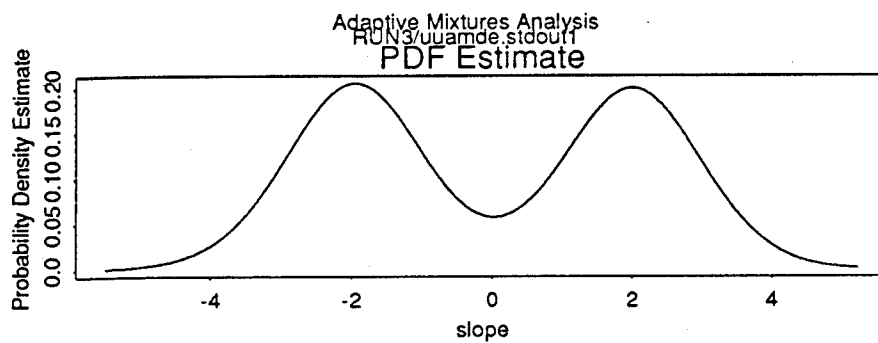
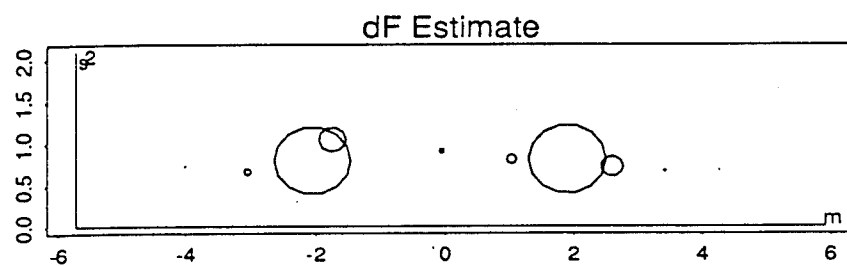


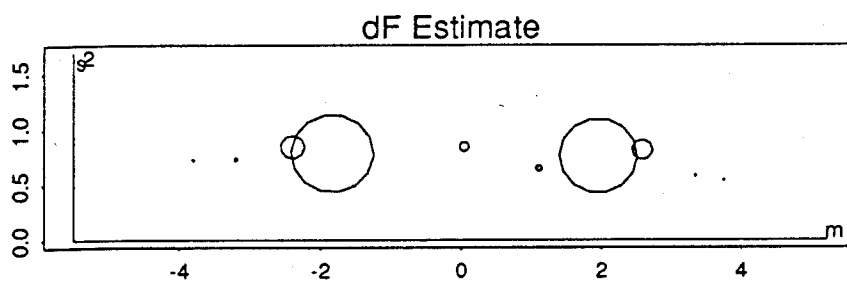
Figure 2



(a)



(b)



Figures 3 a and b.

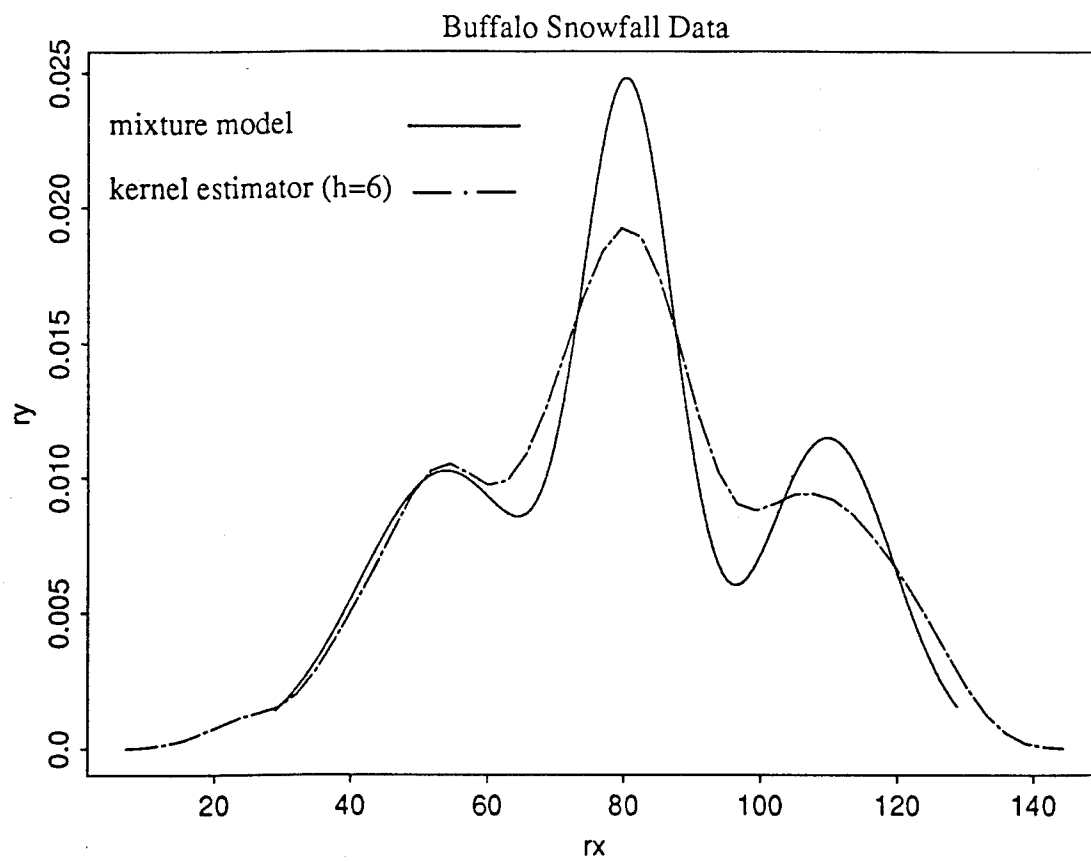


Figure 4a

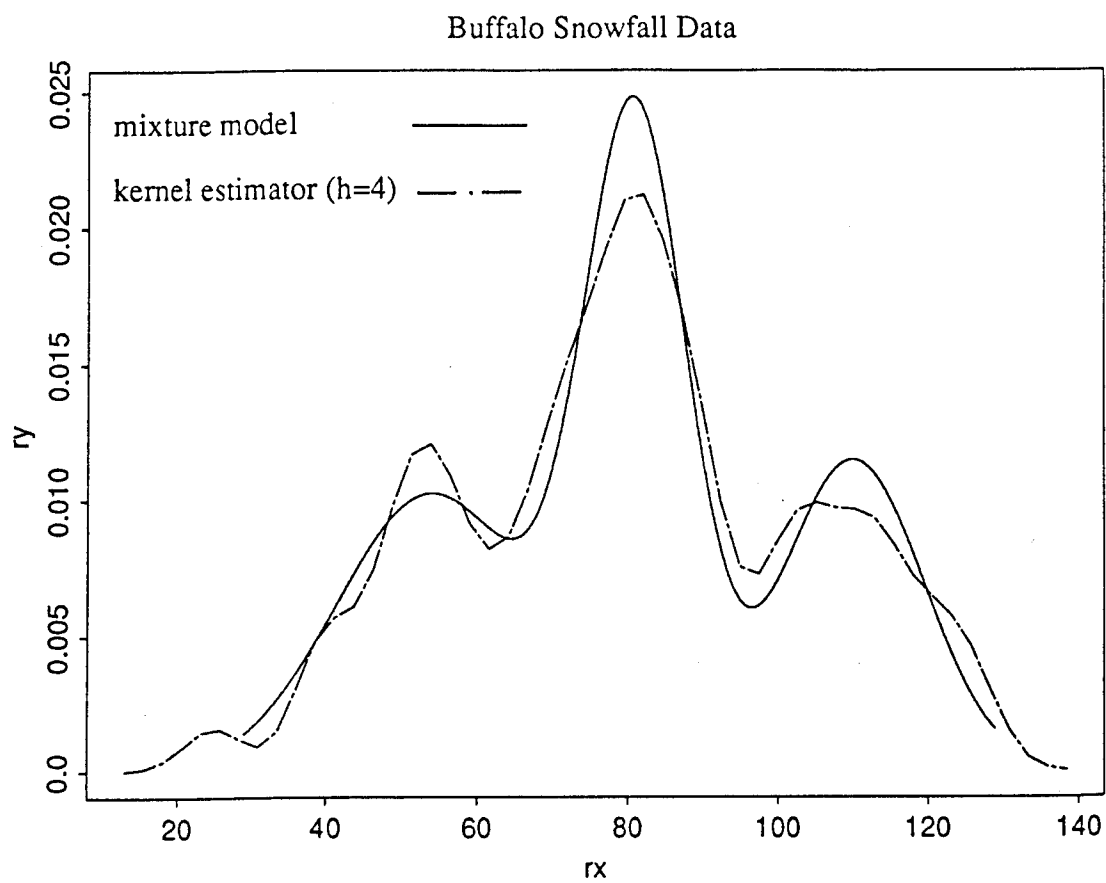
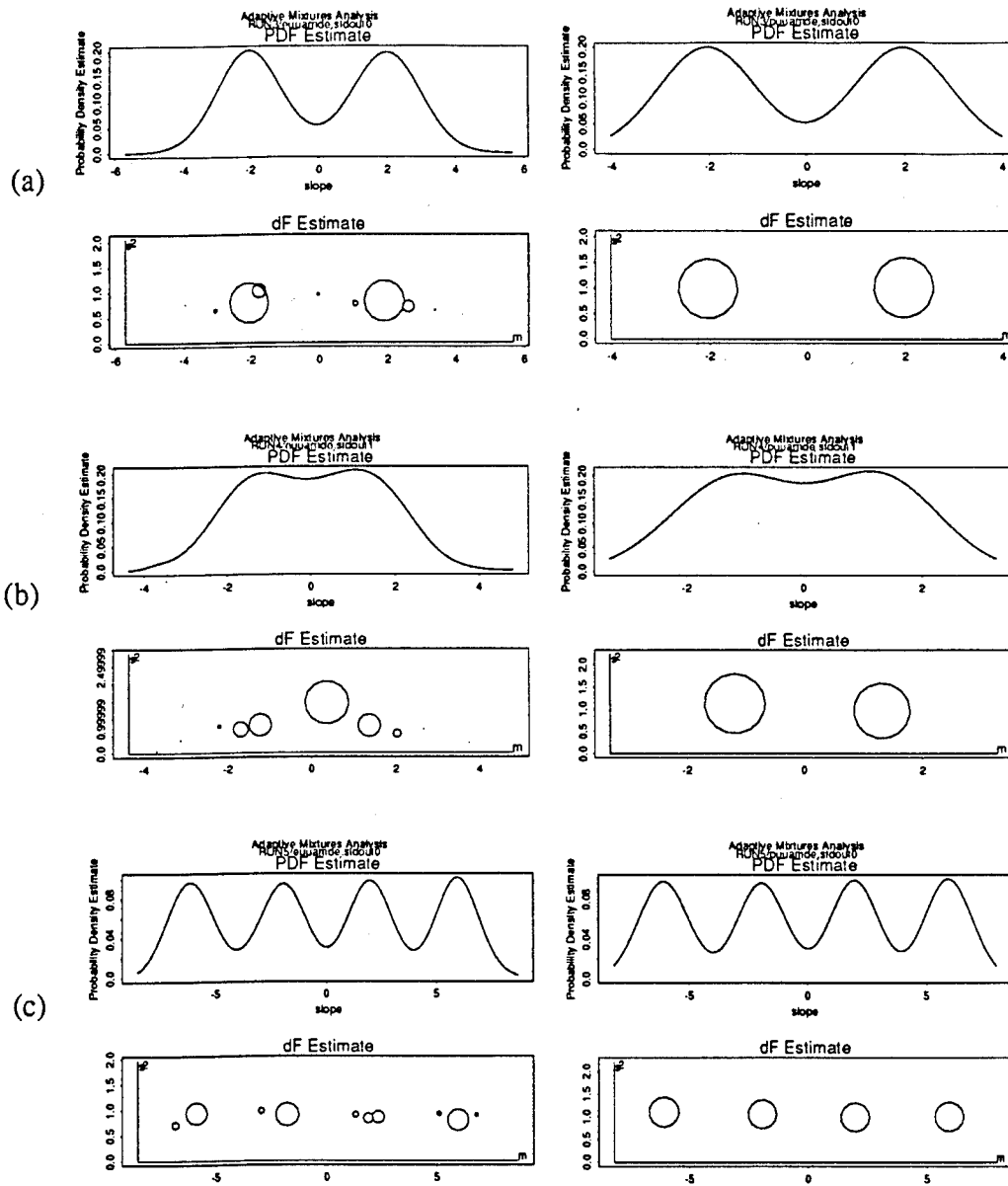


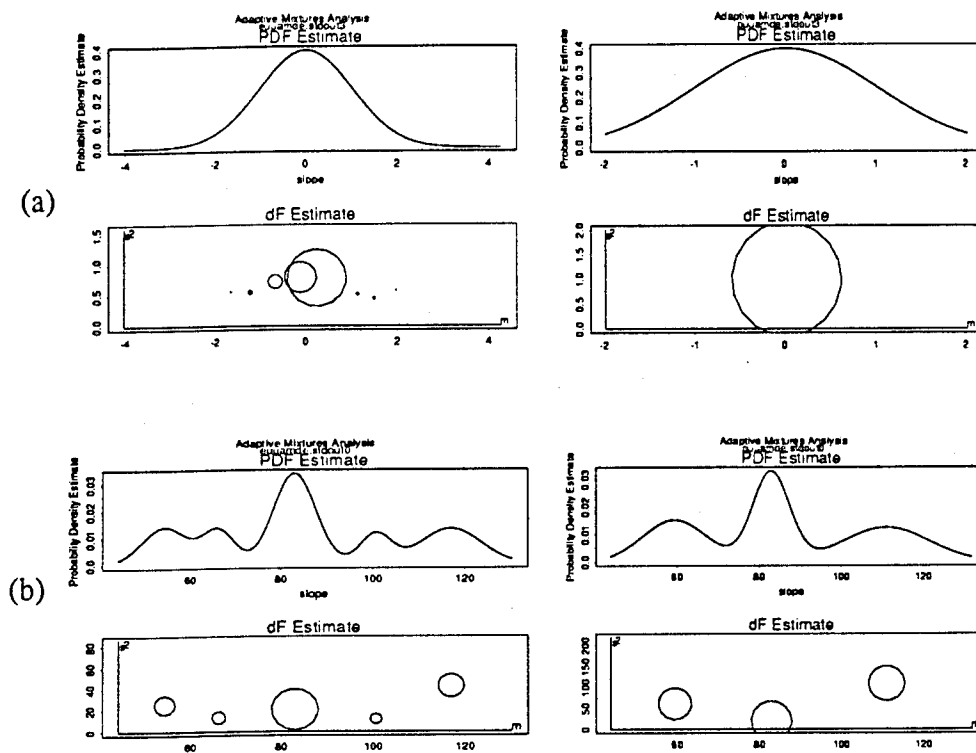
Figure 4b

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Figures 5 a, b, and c.



Figures 6 a and b.

Table 1:

Case/# Terms	1	2	3	4	5	6	7
a - Separated Bimodal		11	4	6	2	2	
b - Bimodal		7	3	6	3	5	1
c - Quadmodal				17	5	3	
d - Standard Normal	3		9	4	4	5	
e - Buffalo Snowfall			4	10	7	4	

Table 2:

Case/# Terms	1	2	3	4	5	6	7
a - Separated Bimodal		.017	.025	.023	.025	.043	
b - Bimodal		.021	.028	.033	.030	.032	.017
c - Quadmodal				.042	.046	.063	
d - Standard Normal	.011		.024	.024	.020	.018	
e - Buffalo Snowfall							

FIGURE AND TABLE CAPTIONS

Figure 1 - Pruning curves for the reduction of a 10 term model to a 2 term model.

Figure 2 Test Cases

(a) - $\alpha(x) = .5 * N(-2, 1) + .5 * N(2, 1)$,

(b) - $\alpha(x) = .5 * N(-1.25, 1) + .5 * N(1.25, 1)$,

(c) - $\alpha(x) = .25 * N(-6, 1) + .25 * N(-2, 1) + .25 * N(2, 1) + .25 * N(6, 1)$,

(d) - $\alpha(x) = N(0, 1)$,

(e) - The Buffalo Snowfall Data

Figures 3 a and b - Adaptive mixtures estimates for two of the resamplings of the data set drawn from case a.

Figures 4 a, b - Comparison of the pruned 3 term model which has been expectation maximized against kernel estimates of the original Buffalo snowfall data with bandwidths of 6. and 4.

Figures 5 a, b, and c - Expectation maximized adaptive mixtures estimates along with the output of the pruning process for the first three cases.

Figures 6 a and b - Expectation maximized adaptive mixtures estimates along with the output of the pruning process for the last two cases.

Table 1: Number of terms for each case.

Table 2: Average L_1 error for each test case for each model complexity.

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